### Dan Lu

Ph.D., Research Scientist III Computational Earth Science Group Oak Ridge National Laboratory (ORNL)

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Education	Ph.D. in Computational Hydrology Florida State University, Tallahassee, FL	2012
	M.S. in Hydrology and Water Resources China University of Geosciences, Beijing, China	2007
	<b>B.S. in Environmental Engineering</b> Hebei University of Geosciences, Shijiazhuang, China	2004
Professional Experience	Staff Research Scientist III Oak Ridge National Laboratory	2019 – Now
	Staff Research Scientist II Oak Ridge National Laboratory	2016 - 2019
	Postdoctoral Research Associate Oak Ridge National Laboratory	2013 - 2016
	Postdoctoral Research Associate U.S. Geological Survey, Menlo Park, CA	2012 - 2013

CURRENT GRANTS ORNL - Laboratory Directed Research & Development, Uncertainty Quantification for AI Models, \$675K for FY22-FY23, PI.

> DOE - Office of Fossil Energy and Carbon Management, Science-informed Machine Learning in Subsurface Applications, \$550K/year for FY22-FY27, PI.

DOE - Water Power Technologies Office, An Uncertainty-Aware, Machine Learning-Enabled Hydropower Seasonal Forecast Model, \$50K for FY23, PI.

DOE - Advanced Scientific Computing Research, Efficient Machine Learning for Leadership Facility Scientific Data Analytics, \$3.4M for FY22-FY24, Task Lead.

DOE - Advanced Scientific Computing Research, Decision and Control of Complex Systems: a Data-Driven Framework, \$4.2M for FY21-FY23, Task Lead.

DOE - Biological and Environmental Research, Advancing Watershed System Understanding through Machine Learning, \$6.2M for FY21-FY23, Task Lead.

**DOE** - Basic Energy Sciences, Machine Learning for Improving Accelerator and Target Performance, \$4.2M for FY21-FY23, Task Lead.

DOE - Biological and Environmental Research, Spruce and Peatland Responses Under Changing Environments, \$8.3M/year for FY20-FY23, Investigator.

PEER-REVIEWED
JOURNAL
PUBLICATIONS

- Bhanja S. N., Coon, E. T., **Lu, D.**, and Painter S. L., Evaluation of distributed process-based hydrologic model performance in diverse catchments using only a priori information, Accepted in Journal of Hydrology, 2023
- Fan, M., **Lu, D.**, Rastogi, D., and Pierce, E.M., *A spatiotemporal-aware climate model ensembling method for improving precipitation predictability*. Journal of Machine Learning in Modeling and Simulation, V3 (4), 29-55, 2022, doi: 10.1615/JMachLearn-ModelComput.2022046715.
- Fan, M., Lu, D., and Liu, S., A deep learning-based direct forecasting of CO2 plume migration. Geoenergy Science and Engineering, https://doi.org/10.1016/j.geoen.2022.211363.
- Fan, M., Zhang, L., Liu, S., Yang, T., and Lu, D., Identifying the hydrometeorological decision factors influencing reservoir releases over the upper Colorado region. Accepted in IEEE International Conference in Data Mining DMESS workshop.
- Liu, S., Lu, D., Ricciuto, D., and Walker A., *Improving net ecosystem CO2 flux prediction using memory-based interpretable machine learning*. Accepted in IEEE International Conference in Data Mining DMESS workshop.
- Lu, D., Painter, S. L., Azzolina, N. A., Burton-Kelly, M., Jiang T., and Williamson C., Accurate and rapid forecasts for geologic carbon storage via learning-based inversion-free prediction, Frontiers in Energy Research, 9: 752185, 2022.
- Gangrade, S., Lu, D., Kao, S., Painter, S., and Coon, E., Machine learning assisted reservoir operation model for long-term water management simulation, J. of the Amer. Water Res. Ass., https://doi.org/10.1111/1752-1688.13060, 2022.
- Radaideh, M., Pappas, C., Walden, C., **Lu, D.**, Vidyaratne, L., Britton, T., Rajput, K., Schram, M., Cousineau, S., *Time series anomaly detection in power electronics signals with recurrent and convlstm autoencoders*, Digital Signal Processing, 130, 103704, https://doi.org/10.1016/j.dsp.2022.103704, 2022.
- **Lu, D.**, Konapala, G., Painter, S., and Kao, S., Streamflow simulation in data-scarce basins using Bayesian and physics-informed machine learning models, Journal of Hydrometeorology, 1421-1438, 2021.
- Huang, X., **Lu, D.**, Ricciuto, D. M., Hanson, P. J., Richardson, A. D., Lu, X., Weng, E., Nie, S., Jiang, L., Hou, E., Steinmacher, I. F., and Luo, Y., *A model-independent data assimilation (MIDA) module and its applications in ecology*, Geoscientific Model Development, 14(8), 5217-5238, 2021.
- Chen, A., Mao, J., Ricciuto, D., **Lu, D.**, Xiao, J., Li, X., Thornton, P. E., and Knapp, A. K., Seasonal changes in GPP/SIF ratios and their climatic determinants across the northern hemisphere, Global Change Biology, 1-12, 2021.
- Zhang, P., Liu, S., **Lu, D.**, Sankaran, R., Zhang, G., *An out-of-distribution-aware autoencoder model for reduced chemical kinetics*, American Institute of Mathematical Sciences Journal, Doi: 10.3934/dcdss.2021138, 2021.

- Walker, A., Johnson, A., Rogers, A., Anderson, J., Bridges, R., Fisher R., **Lu, D.**, Ricciuto, D., Serbin, S. and Ye M., *Multi-hypothesis analysis of photosynthesis models reveals the unexpected influence of empirical assumptions at leaf and global scales*, Global Change Biology, Doi: 10.1111/gcb.15366, 2020.
- Konapala, G., Kao, S., Painter, S., and **Lu, D.**, Machine learning assisted hybrid models can improve streamflow simulation in diverse catchments across the conterminous US, Environmental Research Letter, 15(10), 2020.
- **Lu, D.**, and Ricciuto, D., Efficient surrogate modeling methods for large-scale Earth system models based on machine learning techniques, Geoscientific Model Development, 12, 1791-1807, 2019.
- Mo, S., Shi, X., **Lu, D.**, Ye, M., and Wu, J., An adaptive Kriging surrogate method for efficient uncertainty quantification with an application to geological carbon sequestration modeling, Computers and Geosciences, 125, 69-77, 2019.
- Evans, K., Kennedy, J., **Lu, D.**, Forrester, M. M., Price, S., Fyke, J., Bennett, A., Hoffman, M., Tezaur, I., Zender, C., and Vizcaino, M., *LIVVkit 2.1: Automated and extensible ice sheet model validation*, Geosci. Model Dev., 12, 1067-1086, 2019.
- Walker A. P., Ye, M., **Lu, D.**, De Kauwe, M. G., Gu, L., Medlyn, B. E., Rogers, A., and Serbin, S. P., The multi-assumption architecture and testbed (MAAT v1.0): R code for generating ensembles with dynamic model structure and analysis of epistemic uncertainty from multiple sources, Geoscientific Model Development, 11, 2018.
- **Lu, D.**, D. Ricciuto, M. Stoyanov, and L. Gu, *Calibration of the E3SM land model using surrogate based global optimization*, Journal of Advances in Modeling Earth Systems, 10, 1337–1356, 2018.
- **Lu, D.**, D. Ricciuto, and K. Evans, An efficient Bayesian data-worth analysis using a multilevel Monte Carlo method, Advances in Water Resources, 113, 223–235, 2018.
- Shi, X., S. Finsterle, K. Zhang, and **Lu, D.**, Advances in multiphase flow and transport in the subsurface environment., Geofluids, https://doi.org/10.1155/2018/2906326, 2018.
- Mo, S., Lu, D., X. Shi, G. Zhang, M. Ye, J. Wu, and J. Wu, A Taylor expansion-based adaptive design strategy for global surrogate modeling with applications in groundwater modeling, Water Resources Research, 53, 10802–10823, 2017.
- Lu, D., D. Ricciuto, A. Walker, C. Safta, and W. Munger, Bayesian calibration of terrestrial ecosystem models: a study of advanced Markov chain Monte Carlo methods, Biogeosciences, 14, 4295–4314, 2017.
- Xi, M., Lu, D., D. Gui, Z. Qi, and G. Zhang, Calibration of an agricultural-hydrological model (RZWQM2) using surrogate global optimization, Journal of Hydrology, 544, 2017.
- **Lu, D.**, G. Zhang, C. Webster, and C. Barbier, An improved multilevel Monte Carlo method for estimating probability distribution functions in stochastic oil reservoir simulations, Water Resources Research, 52, 9642–9660, 2016.
- (\*\*\* This work was reported in *The BAKKEN Magazine in 2015* [online version])

- Liu, P., A. S. Elshall, M. Ye, P. Beerli, X. Zeng, Lu, D., and Y. Tao, Evaluating marginal likelihood with thermodynamic integration method and comparison with several other numerical methods, Water Resources Research, 52, 734–758, 2016.
- Hill, M. C., D. Kavetski, M. Clark, M. Ye, M. Arabi, **Lu, D.**, L. Foglia, and S. Mehl, *Practical use of computationally frugal model analysis methods*, Ground Water, 54, 159–170, 2015.
- **Lu, D.**, M. Ye, and G. P. Curtis, Maximum likelihood Bayesian model averaging and its predictive analysis for groundwater reactive transport models, Journal of Hydrology, 529(3), 1859–1873, 2015.
- **Lu, D.**, M. Ye, M. C. Hill, E. P. Poeter, and G. P. Curtis, *A computer program* for uncertainty analysis integrating regression and Bayesian methods, Environmental Modeling & Software, 60, 41–56, 2014.
- Zhang, G., Lu, D., M. Ye, M. Gunzburger, and C. Webster, An adaptive sparse-grid high-order stochastic collocation method of Bayesian inference in groundwater reactive transport modeling, Water Resources Research, 49(10), 6871–6892, 2013.
- Lu, D., M. Ye, P. D. Meyer, G. P. Curtis, X. Shi, X. Niu, and S. B. Yabusaki, *Effects of error covariance structure on estimation of model averaging weights and predictive performance*, Water Resources Research, 49(9), 6029–6047, 2013.
- Hill, M. C., D. Kavetski, M. Clark, M. Ye, and **Lu**, **D.**, Uncertainty quantification for environmental models, SIAM News, 45(9), 2012.
- **Lu, D.**, M. C. Hill, and M. Ye, Analysis of regression confidence intervals and Bayesian credible intervals for uncertainty quantification, Water Resources Research, 48(9), 2012. (\*\*\* This paper was selected as *Editor's Highlight* entitled new insights into faster computation of uncertainties)
- Lu, D., M. Ye, S. P. Neuman, and L. Xue, Multimodel Bayesian analysis of data-worth applied to unsaturated fractured tuffs, Advances in Water Resources, 35, 69–82, 2012.
- Neuman, S. P., L. Xue, M. Ye, and **Lu, D.**, *Bayesian analysis of data-worth considering model and parameter uncertainties*, Advances in Water Resources, 36, 75–85, 2012. (\*\*\* *Top 10 Cited Paper* in 2012-2013 of Advances in Water Resources [Certificate])
- Lu, D., M. Ye, and S. P. Neuman, Dependence of Bayesian model selection criteria and Fisher information matrix on sample size, Mathematical Geoscience, 43, 2011.
- Ye, M., Lu, D., S. P. Neuman, and P. D. Meyer, Comment on "Inverse groundwater modeling for hydraulic conductivity estimation using Bayesian model averaging and variance window" by Frank T.-C. Tsai and Xiaobao Li, Water Resources Research, 46, W02801, 2010.

PEER-REVIEWED CONFERENCE PUBLICATIONS

- **Lu, D.**, Ricciuto, D., and Zhang J., *Invertible neural networks for E3SM land model calibration and simulation*. Proceedings of ICLR AI for Earth and Space Sciences Workshop, 2022.
- Lu, D., Ricciuto, D., and Liu, S., An interpretable machine learning model for ad-

- vancing terrestrial ecosystem predictions. Proceedings of ICLR AI for Earth and Space Sciences Workshop, 2022.
- Radaideh, M., Pappas, C., Lu, D., Walden, J., Cousineau, S., Britton, T., Rajput, K., Vidyaratne, L., Schram, M., *Progress on machine learning for the SNS high voltage converter modulators*, North American Particle Accelerator Conference, 2022.
- Bororwiec, K., **Lu, D.**, Chandan, V., Chatterjee, S., Ramuhalli, P., Tipireddy, R., Halappanavar, M., and Liu, F., *Bi-fidelity weighted transfer learning for efficient heat transfer model simulation*, IEEE International Conference on Machine Learning and Applications, 2022.
- Tran, H., Lu, D., and Zhang, G., Exploiting the local parabolic landscapes of adversarial losses to accelerate black-box adversarial attack, European Conference on Computer Vision (ECCV), 2022.
- Fan, M., Lu, D., and Rastogi, D., Multimodel ensemble predictions of precipitation using Bayesian neural networks. Proceedings of ICLR AI for Earth and Space Sciences Workshop, 2022.
- Liu, S., Zhang, P., **Lu, D.**, and Zhang, G., *PI3NN: Out-of-distribution-aware prediction intervals from three neural networks.* Proceedings of International Conference on Learning Representations (ICLR), 2022.
- Lu, D., Pierce, E., Kao, S., Womble, D., Li, L., Rempe, D., Machine learning-enabled model-data integration for predicting subsurface water storage. Proceedings of NeurIPS Tackling Climate Change with Machine Learning workshop, 2021.
- **Lu, D.**, Painter, S., Azzolina N., and Burton-Kelly M., Accurate and timely forecasts of geologic carbon storage using machine learning methods. Proceedings of NeurIPS Tackling Climate Change with Machine Learning workshop, 2021.
- Pappas, C., Lu, D., Schram, M., and Vrabie D., Machine learning for improved availability of the SNS klystron high voltage converter modulators, 12th Int. Particle Acc. Conf. doi:10.18429/JACoW-IPAC2021-THPAB252, 2021.
- Zhang, P., Liu, S., Lu, D., and Zhang, G., A prediction interval method for uncertainty quantification of regression models, Proceedings of ICLR Workshop on Deep Learning for Simulation, 2021.
- Tran, H., **Lu**, **D**., and Zhang, G., *Boosting black-box adversarial attack via exploiting loss smoothness*, Proceedings of ICLR Workshop on Security and Safety in Machine Learning Systems, 2021.
- Zhang, J., Tran, H., **Lu, D.**, and Zhang, G., *Enabling long-range exploration in mini*mization of multimodal functions, Proceedings of Conference on Uncertainty in Artificial Intelligence (UAI), 2021.
- **Lu, D.**, and Ricciuto D., Efficient distance-based global sensitivity analysis for terrestrial ecosystem modeling, Proceedings of the 2020 IEEE International Conference on Data Mining Workshops, Doi: 10.1109/ICDMW51313.2020.00052, 2020.

**Lu, D.**, Liu S., and Ricciuto D., An efficient Bayesian method for advancing the application of deep learning in earth science. Proceedings of the 2019 IEEE International Conference on Data Mining Workshops, Doi: 10.1109/ICDMW.2019.00048, 2019.

Lu, D., and Ricciuto D., Learning-based inversion-free model-data integration to advance ecosystem model prediction. Proceedings of the 2019 IEEE International Conference on Data Mining Workshops, Doi: 10.1109/ICDMW.2019.00049, 2019.

Zhang, G., Lu, D., M. Ye, M. Gunzburger, and C. Webster, An efficient surrogate modeling approach in Bayesian uncertainty analysis, 11th International Conference of Numerical Analysis and Applied Mathematics, 1558, 898–901, 2013.

Ye, M., Lu, D., S. P. Neuman, and L. Xue, Multimodel Bayesian analysis of dataworth applied to unsaturated fractured tuffs, International Conference on Groundwater: Our Source of Security in an Uncertain Future, Pretoria, South Africa, 2011.

Lu, D., M. C. Hill, and M. Ye, Analysis of regression and Bayesian predictive uncertainty measures, MODFLOW and More 2011 Conference, Golden, CO, 2011.

Neuman, S. P., L. Xue, M. Ye, and **Lu, D.**, *Multimodel assessment of the worth of data under uncertainty*, Water Management Symposium, Phoenix, AZ, 2011.

Ye, M., Lu, D., G. Miller, G. P. Curtis, P. D. Meyer, and S. B. Yabusaki, Assessment of predictive uncertainty in coupled groundwater reactive transport modeling, Conference on Goldschmidt – Earth, Energy and Environment, Knoxville, TN, 2010.

#### TECHNICAL REPORTS

Barbier, C., **Lu, D.**, N. Collier, F. Curtis, C. G. Webster, and Y. Polsky, *High performance computing simulations for shale gas formation flow transport and uncertainty quantification analysis*, ORNL Technical Report, ORNL/TM-2015/543, 2015.

### SOFTWARE DEVELOPMENT

UCODE\_2014: A Computer Code for Sensitivity Analysis, Model Calibration, and Uncertainty Evaluation

Sponsor: U.S. Geological Survey

Developers: Eileen P. Poeter, Mary C. Hill, Dan Lu, and Steffen Mehl

Webpage: http://igwmc.mines.edu/freeware/ucode/

PI3NN: A Computer Code for Uncertainty Quantification of Machine Learning Model Predictions

Sponsor: Oak Ridge National Laboratory AI Initiative Developers: Siyan Liu, **Dan Lu**, and Guannan Zhang Webpage: https://github.com/liusiyan/PI3NN

# LECTURES IN SHORT COURSES

Uncertainty Quantification In Earth System Modeling, Department of Mathematics at the Federal University of Parana (UFPR), Brazil virtually, June, 2021.

MODFLOW, with the GIS-based GUI FREEWAT and Calibration and Uncertainty Quantification Using UCODE, Colorado School of Mines, Golden, CO, 2017.

Groundwater Model Calibration Using OSTRICH: with Presentation of Additional Capabilities Available using PEST, PEST++ and UCODE-2014, Colorado School of

Mines, Golden, CO, 2015.

## SELECTED ORAL PRESENTATIONS

Uncertainty quantification of machine learning models in scientific and engineering applications, PNNL, Oct. 25-26, 2022.

Uncertainty quantification of machine learning models to improve streamflow prediction in changing climate and environmental conditions, AGU Fall meeting, Dec., 2022.

(Invited) Machine learning for improving earth system predictability, SIAM Conference on Mathematics of Planet Earth (MPE22), July 2022.

(Invited) PI3NN-LSTM: improving machine learning model prediction of streamflow in novel climate conditions, HydroML workshop, May 2022.

(Invited) ML4UQ: machine learning to enable efficient uncertainty quantification in climate models, SIAM Conference on Uncertainty Quantification (UQ22), April 2022

(Invited) Physics-informed, interpretable machine learning for terrestrial ecosystem predictions, 11th International Conference on Ecological Informatics, November 2021.

(Invited) A prediction interval method for uncertainty quantification of regression models, Ecological Society of America Annual Meeting, August 2021.

(Invited) Machine learning methods for improving terrestrial ecosystem predictions, Society for Industrial and Applied Mathematics Annual Meeting, July 2021.

(Invited) An efficient bayesian machine learning method for advancing ecological forecasting, Ecological Society of America Annual Meeting, August 2020.

(Invited) An efficient Bayesian method for advancing the application of deep learning in earth science in ICDM conference, Beijing, China, November 2019.

(Invited) Learning-based inversion-free model-data integration to advance ecosystem model prediction in ICDM conference, Beijing, China, November 2019.

(Invited) 2nd workshop on quantifying and reducing uncertainty in Earth system model projections, University of Leeds, UK, 2019.

(Invited) Efficient surrogate modeling methods to advance model-data integration, American Geophysics Union annual meeting, Washington D.C., 2018.

(Invited) Optimization of sensor networks for improving climate predictions, DOE-BER headquarter, Germantown, Maryland, 2018.

(Invited) A systematic Bayesian uncertainty quantification framework in environmental modeling, Jinan University, Guangzhou, China, 2018.

(Invited) Efficient surrogate modeling methods for model-data integration, Geological Survey of Japan, AIST, Japan, 2018.

(Invited) Efficient uncertainty quantification methods in groundwater contaminant risk assessment, Japan Geosciences Union Annual Meeting, Chiba, Japan, 2018.

(Invited) Application of reduced-order modeling techniques for uncertainty quantification, CSMD-CSED Cross-Divisional Seminar, 2018.

(Invited) Potential exascale applications for quantifying uncertainty in the land-atmosphere system, Exascale Application in Climate and Environmental Science workshop, 2018.

(Invited) Advance climate model development, prediction, and risk assessment using artificial intelligence, AI for Climate Sciences Seminar, 2018.

An efficient Bayesian data-worth analysis using a multilevel Monte Carlo method, American Geophysics Union Annual Meeting, New Orleans, LA, 2017.

Quantum behaved particle swarm optimization for parameter estimation in terrestrial ecosystem models, 2017 ESS PI Meeting, Washington D.C., 2017.

Calibration of the Community Land Model (CLM4.5) using surrogate based global optimization, American Geophysics Union Annual Meeting, San Francisco, CA, 2016.

A systematic Bayesian framework for uncertainty quantification in environmental modeling, Earth System Modeling Workshop, Oak Ridge National Laboratory, TN, 2015.

Multilevel Monte Carlo method with application to uncertainty quantification in oil reservoir simulation, American Geophysics Union Annual Meeting, CA, 2014.

Assessment of predictive performance of Bayesian model averaging in groundwater reactive transport models, SIAM Conference on Uncertainty Quantification, GA, 2014.

Maximum likelihood Bayesian model averaging of groundwater reactive transport models, 2014 SIAM SEAS Annual Meeting, Melbourne, FL, 2014.

Integration of Markov chain Monte Carlo simulation into UCODE for Bayesian uncertainty analysis, Geological Society of America Annual Meeting, Charlotte, NC, 2012.

Effects of temporal error correlation on quantification of predictive uncertainty in ground-water reactive transport modeling, annual PI meeting of the Subsurface Biogeochemical Research Program of the Department of Energy, Washington D.C., 2012.

Effects of temporal residual correlation on model weights, American Geophysics Union Annual Meeting, San Francisco, CA, 2011.

Multimodel Bayesian analysis of data-worth applied to unsaturated fractured tuffs, Geosciences Applications Opening Workshops on Uncertainty Quantification, NC, 2011.

Analysis of predictive uncertainty measures of regression and Bayesian, 2011 MOD-FLOW and More Meeting, Golden, CO, 2011.

A controlled experiment for investigating prediction accuracy and prediction uncertainty in groundwater flow modeling, American Geophysics Union Annual Meeting, San Francisco, CA, 2010.

Honors and Awards

Distinguished Scientific Achievement Award in ORNL, 2022.

Selected Early Career Scientist to DOE-BER headquarter for the annual meeting, 2018.

Student Travel Fellowship to the annual PI meeting of the subsurface biogeochemical research program of the Department of Energy, 2012.

Statistical and Applied Mathematical Sciences Institute (SAMSI) Travel Award to the geosciences applications opening workshops on uncertainty quantification, 2011.

Graduate Student Scholarship for Academic Excellence, China University of Geosciences, China, 2004–2007.

Excellent Undergraduate Student of Hebei Province, China, 2003.

Undergraduate Student Scholarship for Academic Excellence, Hebei University of Geosciences, China, 2000–2004.

Organizing committees

Groundwater Technique Committee for American Geophysics Union, 2016 – Now.

Program Committee for Tackling Climate Change with Machine Learning Workshop

at NeurIPS Conference, 2022.

Program Committee for AI for Robust Engineering and Sciences Workshop, 2021-2022. Program Committee for Climate and Weather Domain of PASC19 Conference, 2019.

Supervising Postdocs Dr. Siyan Liu Dr. Ming Fan

EDITORIAL SERVICES Topical Editor: Geoscientific Model Development, 2021–Present

Associate Editor: Artificial Intelligence for the Earth Systems, 2021–Present

Associate Editor: Frontiers in Water, 2022–Present

Editor: Special issue on data-driven machine learning for advancing hydrological and hydraulic predictability, Frontiers in Water, 2022, co-organized with Yang, T., and Liu, X.

Co-editor: Special issue on advances in multiphase flow and transport in the subsurface environment, **Geofluids**, https://doi.org/10.1155/2018/2906326, 2018, co-organized with Shi, X., S. Finsterle, K. Zhang.

Memberships

Society for Industrial and Applied Mathematics (SIAM)

American Geophysical Union (AGU) Geologic Society of America (GSA)